along the ⟨100⟩ directions, with a Cr–C distance of about 2·12 Å. The interatomic distances are listed in Table 2. The Cr coordination about the carbon atom is an 8-fold square anti-prism, with the carbon atom displaced slightly from the center.

The compounds which form in this structure type have been reviewed recently (Stadelmaier, 1969). They include $Cr_{23}C_6$, $Mn_{23}C_6$, and many ternary carbides and borides.

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For estriol, $\varphi_{200}=0$.

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It is shown that the value of the important phase φ_{200} for estriol is zero.

The estriol structure ($C_{18}H_{24}O_3$, $P2_1$, $Z=4$) was the first to be solved *via* the least-squares analysis of the cosine invariants (Hauptman, Fisher, Hancock & Norton, 1969). The phase $\varphi_{200}=0$ was one of five in the basic set but its value was not unambiguously determined by means of $\sum_1$. Nevertheless its value was well determined by 'an argument which the reader is challenged to supply and which depends on the facts that $|E_{200}|=5{\cdot}40$, $|E_{100}|=0{\cdot}00$, and that there are two molecules in the asymmetric unit'. Since the appearance of this challenge no one has responded to it, but some have questioned the existence of such an argument (*e.g.* Woolfson, 1971, p. 428). It therefore seems appropriate to present this brief analysis, especially since it may well have more general applicability.

First, the fact that the low angle $|F_{100}|^2$ was measured to be zero (not merely small) must surely have a fundamental structural significance. Next, ignoring the negligible contribution of the hydrogen atoms,

$$E_{200}=\frac{2}{\sqrt{84}}\sum_{\mu=1}^{42}\cos 4\pi x_\mu\,, \tag{1}$$

where the x_μ are the x coordinates of the 42 independent nonhydrogen atoms. Only if either

$$x_\mu=0 \text{ or } \tfrac{1}{2},\ \mu=1,\ldots,42\,, \tag{2}$$

or

$$x_\mu=\pm\tfrac{1}{4},\ \mu=1,\ldots,42\,, \tag{3}$$

would $|E_{200}|$ attain the maximum possible value of $84^{1/2}\simeq 9{\cdot}17$. However $|E_{200}|$ is in fact equal to 5·40, large enough to imply that either (2) holds or (3) holds, approximately. Since there are two independent molecules, each approximately planar, in the asymmetric unit, it readily follows that either

$$\left.\begin{aligned} &x_\mu=\varepsilon_\mu,\ \mu=1,\ldots,21;\ \text{molecule I,}\\ &x_\mu=\tfrac{1}{2}+\varepsilon_\mu,\ \mu=22,\ldots,42;\ \text{molecule II,}\end{aligned}\right\} \tag{4}$$

or

$$\left.\begin{aligned} &x_\mu=\tfrac{1}{4}+\varepsilon_\mu,\ \mu=1,\ldots,21;\ \text{molecule I,}\\ &x_\mu=-\tfrac{1}{4}+\varepsilon_\mu,\ \mu=22,\ldots,42;\ \text{molecule II,}\end{aligned}\right\} \tag{5}$$

where the magnitudes of most of the ε_μ are small.

Next,

$$E_{100}=\frac{2}{\sqrt{84}}\sum_{\mu=1}^{42}\cos 2\pi x_\mu \tag{6}$$

and, according as (4) or (5) holds, either

$$E_{100}\simeq\frac{2}{\sqrt{84}}\left\{\sum_{\mu=1}^{21}\left(1-\frac{\varepsilon_\mu^2}{2}\right)-\sum_{\mu=22}^{42}\left(1-\frac{\varepsilon_\mu^2}{2}\right)\right\} \tag{7}$$

or

$$E_{100}\simeq\frac{2}{\sqrt{84}}\left\{\sum_{\mu=1}^{21}\varepsilon_\mu-\sum_{\mu=22}^{42}\varepsilon_\mu\right\}, \tag{8}$$

i.e. either

$$E_{100}\simeq-\frac{1}{\sqrt{84}}\left\{\sum_{\mu=1}^{21}\varepsilon_\mu^2-\sum_{\mu=22}^{42}\varepsilon_\mu^2\right\}, \tag{9}$$

or

$$E_{100}\simeq\frac{2}{\sqrt{84}}\left\{\sum_{\mu=1}^{21}\varepsilon_\mu-\sum_{\mu=22}^{42}\varepsilon_\mu\right\}. \tag{10}$$

Taking into account the fact that the magnitudes of the ε_μ are small, inspection of (9) and (10) clearly shows that it is (9), rather than (10), which is consistent with the observed value of zero for $|E_{100}|$. It follows that (4), not (5), holds so that (1) implies

$$E_{200}>0 \tag{11}$$

or

$$\varphi_{200}=0\,. \tag{12}$$

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